Lee-Yang edge singularities on the Lattice : Study of singularities in QCD 2+1(fℓ) in the complex μ_B plane using Padé approximants

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Based on work with
Bielefeld-Parma collaboration : in preparation
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July 27 2021

LATTICE 21
JULY 26-30 2021, ZOOM/GATHER@MIT

This project has received funding from the European Union's Horizon 2020 research and Innovation programme under the Marie Skłodowska-Curie grant agreement No. 813942

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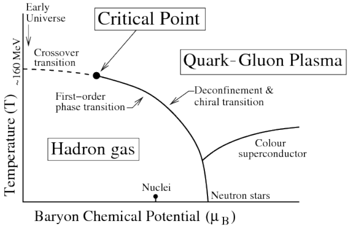
The Goal : Singularities in the QCD phase diagram

- The QCD phase diagram ***remains one of the more important open problems in HEP***. QCD being strongly interacting is best studied using non-perturbative tools.
- ***Lattice QCD*** is currently one of those tools - ***but it only works at zero chemical potential (μ_B=0)***.
- Standard ***MC simulations fail at $\mu_B >$ 0 as the fermion determinant becomes complex***.



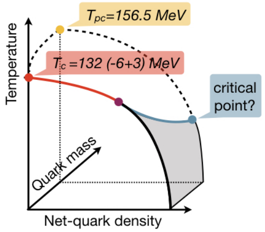


Figure: conjectured QCD phase diagram [1]

[1] left : TIFR-TH-14-11 arXiv:1404.3294 and right : Bielefeld (taken from C.Schmidt)

Current methods to probe the QCD phase diagram on the Lattice

- Taylor expansion about μ_B=0. Simulations get harder for computing higher cumulants. [Allton, et.al Bielefeld-Swansea (2002)]
- Analytic continuation from simulations at imaginary μ_B. (No sign problem in this regime!) [de Forcrand, Philipsen (2002)], [D'Elia and Lombardo, (2002)]
- Recently new methods of resummation have appeared
  - [Mondal et.al arXiv:2106.03165],
  - [Gokce Basar arXiv:2105.08080],
  - [Karthein, et.al Eur. Phys. J. Plus 136, 621 (2021)]
  - [Attila Pásztor et.al Phys. Rev. D 103, 034511] (also based on Padé - similar approach but different goal)

Our approach can be thought of as a combination of the Taylor expansion and analytic continuation methods.

The motivation

- In the Taylor expansion approach at $\mu_B = 0$ we have to ***live with low order cumulants***.
- Also, when sampling at imaginary μ, it gets harder to extract the signal when sampling higher cumulants, ***the result of which is that we have information of low order Taylor series but at multiple points on the Im[μ_B] axis***.

The idea is to use these Tayor coefficients to build a (rational) Padé approximant.

The motivation

- It is no surprise that for ***some classes of functions*** - given the same information - a rational function approximates better than a polynomial. This can be seen very easily for functions ***with poles, branch cuts*** etc.
- But an even more important motivation is ***the recovery of singularities of a function using rational functions***.

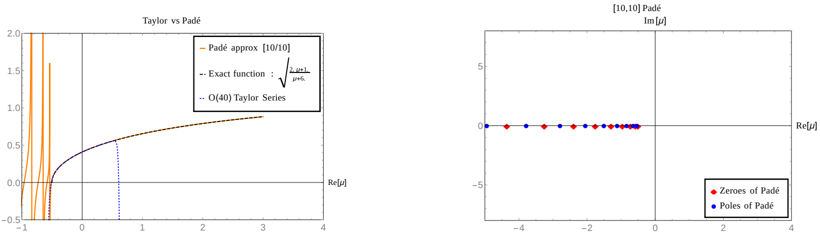


Figure: Failure of Taylor series for a function with a branch cut.

Can we do better? : Multi-Point Padé approximants

- The traditional ***single point Padé*** usually requires many Taylor coefficients even to get a small order rational function!

$$f(x) = \sum_{i=0}^{L} c_i\, x^i + \mathcal{O}(x^{L+1}) \approx R_n^m(x) = \frac{P(x)}{1+Q(x)} = \frac{\sum\limits_{i=0}^{m} a_i\, x^i}{1 + \sum\limits_{j=1}^{n} b_j\, x^j}$$

- Multiple (even low order!) Taylor expansions give us a ***multi-point Padé*** approximant!
  - Linear solver (approximation through order type) (Parma)
  - Generalised χ^2 - (Parma)
  - Remez algorithm (Bielefeld)

Some examples of success :

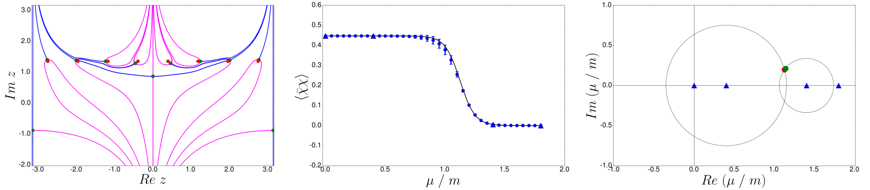


Figure: Thirring (0+1D)[F.dR.,K.Z.,S.S.,Phys.Rev.D 103 (2021) 3, 034513]

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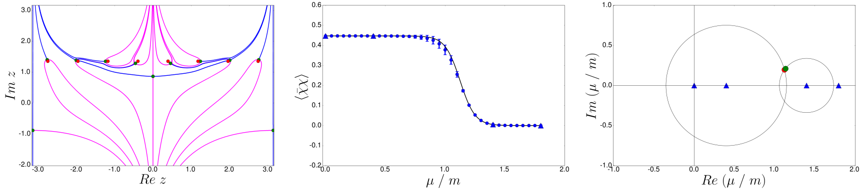

Figure: Thirring (0+1D)[F.dR.,K.Z.,S.S.,Phys.Rev.D 103 (2021) 3, 034513]

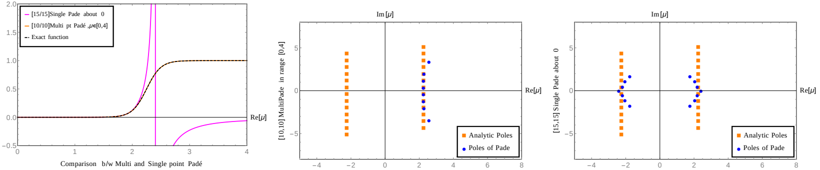

Figure: Left: multi-point vs single Padé approximating the function. (Middle) : Reconstruction of the analytic poles by the multi-point Padé and Bottom (Right) : and by the single point Padé

Observations on multi-point Padé (MP) based on numerical experiments

- ***Poles and other singularities obtained from an MP is interval sensitive***[2]. This means that, even though the closest singularity is usually observed with this approach - we maybe more (or less) sensitive to certain zeroes or poles depending on where we sample the Taylor coefficients.
- Padé theory dictates that a ***genuine pole of the function will remain stable when changing order of the Padé.*** While this is true for clean data (functions without noise) - the picture changes when we introduce noise. [Essentials of Padé approximants - G.A Baker]
- In the presence of noise we are still sensitive to the closest singularity w.r.t. the axis we expand about. ***The only catch being that now the pole moves about roughly in an elipse the size of the magnitude of error introduced***.

[2] plots of test functions in backup slides

A small note on spurious poles...

It is not uncommon in Padé approximations to encounter spurious poles - even when approximating clean data - but these are not all that harmful! They come in mainly the following three forms :

* ***Exactly cancelling pairs of zeroes and poles of the rational function*** - so no need to worry!
* ***Isolated poles which move about wildly*** while changing order - usually move away to infinity when increasing order (eg If simulate an analytic function)
* Simulating noisy data on the other hand can lead to a zero-pole structure in which ***the genuine pole is quasi-stable and moreover the "exactly-cancelling" zero-pole pairs don't exactly cancel anymore!*** The separation between them is of the order of the magnitude of error introduced!

2+1 flav LQCD with imaginary μ

- The idea is to take 2+1 QCD at imaginary chemical potential, ***to see if we can gain information about its singularity structure in the complex μ_B plane***.
- The partition function gets a ***non-trivial periodicity (Roberge-Weiss symmetry):*** $Z(\mu_B + i2\pi T) = Z(\mu_B)$
- The partition also has an additional charge conjugation symmtery under : $\mu_B \to -\mu_B$
- At $\mu_B = i\pi T$ there is an ***expectation of a first order phase transition at all temperatures above the Roberge-Weiss critical end point*** T_{RW}. [A. Roberge and N. Weiss, Nuc. Phys B275 (1986) 734]

2+1 flav LQCD with imaginary μ

- Since the (imaginary) baryon density is expected to become discontinuos above $T > T_{RW}$ [Borsanyi et al, J. High Energ. Phys. 2018, 205 (2018)],the physical observable we are interested to study is the baryon number density $\hat{\mu}_B = \mu_B/T$:

$$\chi_B^1(T, \hat{\mu}_B) = \frac{n_B(T, \hat{\mu}_B)}{T^3} = \frac{\partial(p(T, \hat{\mu}_B)/T^4)}{\partial \hat{\mu}_B}$$

- Because of the symmetries of the partition function mentioned above - $\chi_B^1(T, \hat{\mu}_B)$ is an ***odd, periodic function of*** μ_B/T ***when continued to imaginary chemical potential***.

[3] J.Goswami, F.Karsch, A.Lahiri, M.Neumann and C.Schmidt, PoS CORFU2018 (2019), 162 doi:10.22323/1.347.0162 [arXiv:1905.03625 [hep-lat]].

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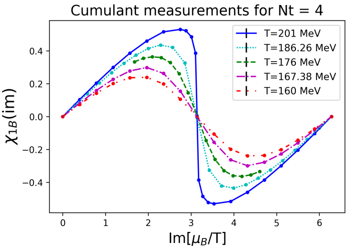
- Because of the symmetries of the partition function mentioned above - $\chi_B^1(T, \hat{\mu}_B)$ is an ***odd, periodic function of*** μ_B/T ***when continued to imaginary chemical potential***.
- Taylor expansions were obtained upto $O((\mu_B/T)^4)$ at various μ_B values shown below.Also, HISQ action was used with $m_s/m_l = 27$ and $\frac{\mu_B}{3} = \mu_\ell = \mu_s$ and T$_{RW}$=201 MeV [3]

[3] J.Goswami, F.Karsch, A.Lahiri, M.Neumann and C.Schmidt, PoS CORFU2018 (2019), 162 doi:10.22323/1.347.0162 [arXiv:1905.03625 [hep-lat]].

Our Lattice setup

$N_\sigma^3 \times N_\tau$	T [MeV[4]]				
$24^3 \times 4$	160	167.38	176	186.26	201
num confs	5550	6000 (12K)	$\sim$ 2500	2500	5000 (11K)
$36^3 \times 6$	125	145			
num confs	5280	8000			



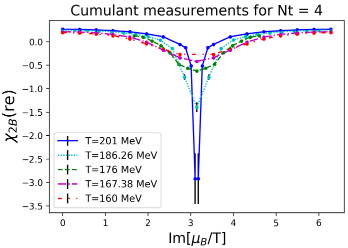


Figure: Left : χ_{1B} and Right : χ_{2B} for N$_\tau$=4 plotted as fiunctions of μ and T

[4] A.Bazavov, T.Bhattacharya, M.Cheng, C.DeTar, H.T.Ding, S.Gottlieb, R.Gupta, P.Hegde, U.M.Heller and F.Karsch, et al. Phys. Rev. D 85 (2012), 054503 doi:10.1103/PhysRevD.85.054503

Higher order cumulants for N_τ=4

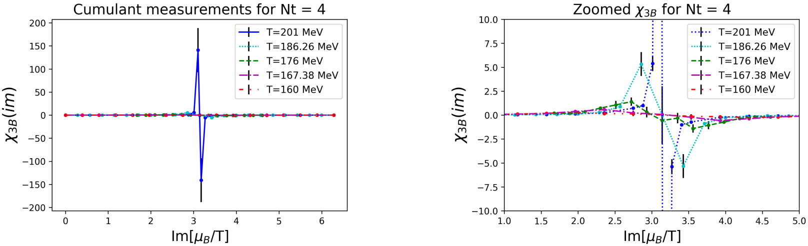


Figure: Left : χ_{3B} and Right : Zoomed χ_{3B} for N_τ=4 plotted as fiunctions of μ and T

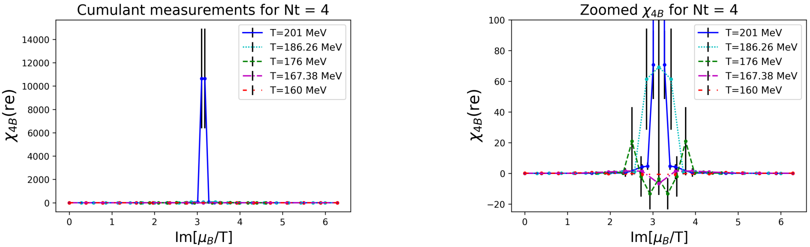


Figure: Left : χ_{4B} and Right : Zoomed χ_{4B} for N_τ=4 plotted as fiunctions of μ and T

Cumulant measurements for N_τ=6, N_σ=36

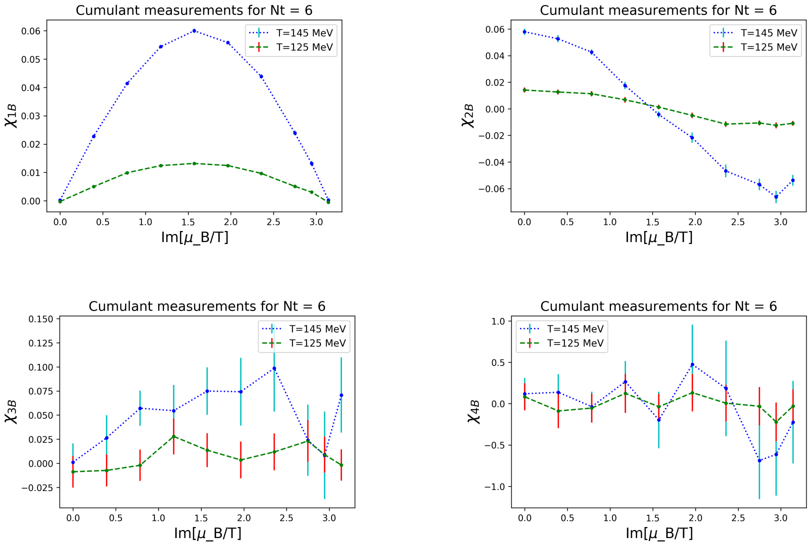


Figure: N_τ = 6 cumulants - better statistics needed!

Singularity structure for RW point N_τ=4

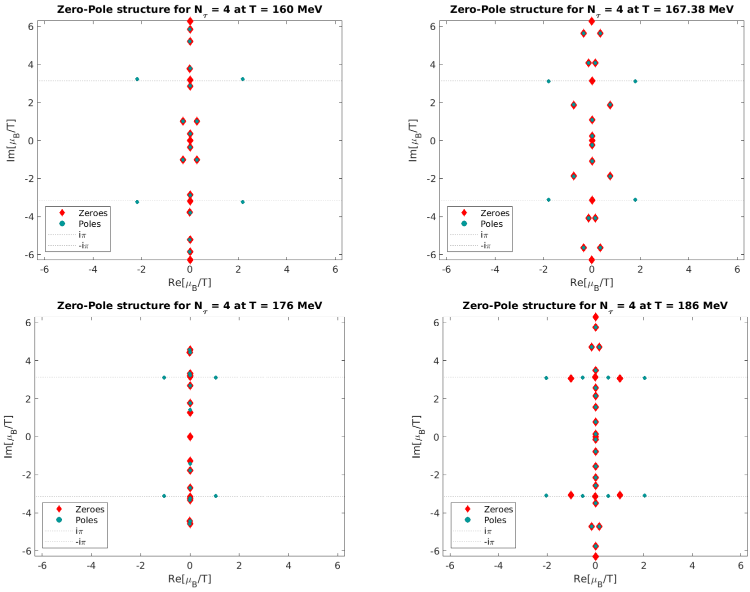


Figure: Zero-Pole structure from Multi-point Padé in the interval $\mu \in [0, 2\pi\iota]$

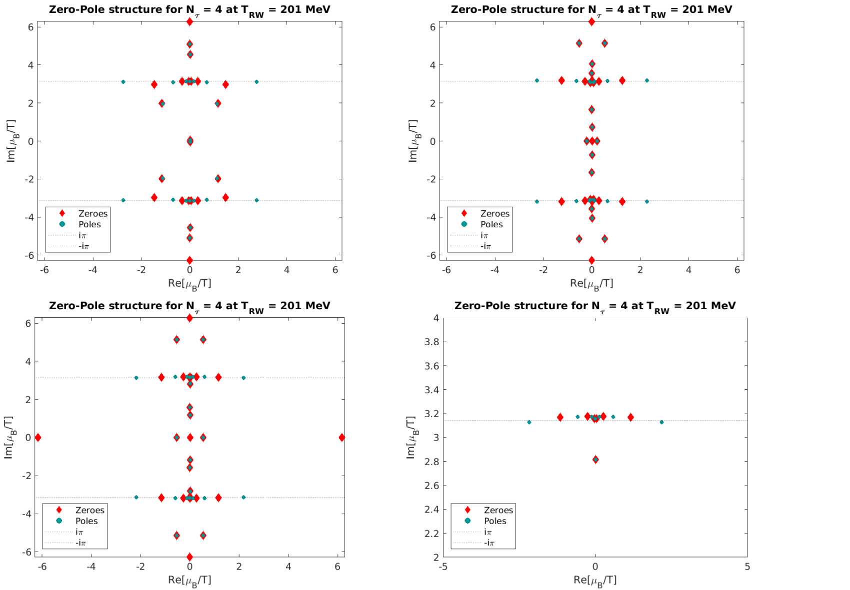


Figure: Zero-Pole structure for T_{RW} from Multi-point Padé in the interval $\mu \in [0, 2\pi\iota]$ for varying choices of points

How the approximations look like for N$_\tau$=4 to extract errorbars

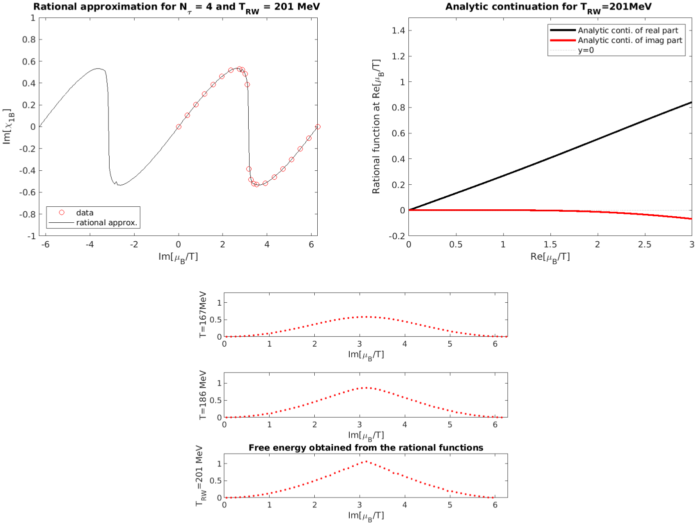
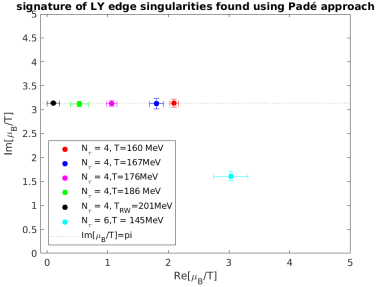


Figure: Approximations for N$_\tau$=4.TOP (L) : Rational approx. to Imag baryon number density, TOP (R) : the corresponding analytic continuation at Re[μ_B/T], BOTTOM : Free energy profile from the integration of rational functions at 3 temperatures.

Bootstrapping the poles with Gaussian noise for $N_\tau = 4$ data



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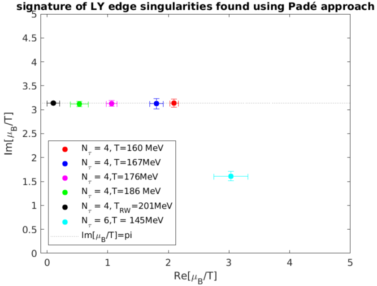


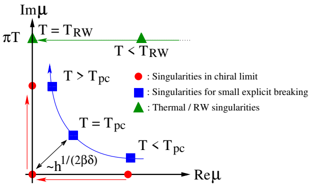


Figure: LEFT : Results from our approach , RIGHT : Complex Singularities [Gábor András Almási et.al Phys. Rev. D 100, 016016 – Published 29 July 2019]

Conclusions and Outlook

- We saw the ***power of Padé approximants to recognize singularities - and also differentiate between the types of singularities***. Moreover, if we are stuck in a scenario with less Taylor coefficients but at multiple points in an interval, ***a Multi-Padé provides a good approximation for the function and also a good estimate of the singularities in that interval.***
- In studying QCD at imaginary chemical potential, ***we seem to find the signature of the RW singularity using ("stable")poles of the Padé approximant***. Other singularities (T_{pc}) need further investigation. More on the scaling of these poles in the next talk by G. Nicotra.
- The runs (generation and measurements codes) were performed between Marconi100 (Cineca Bologna, ISCRA C project and INFN computing time) by K.Zambello in Parma and Jülich Supercomputing Centre (JSC) (Germany) by the Bielefeld group.

***********end***********

BACK-UP SLIDES!!

Interval dependence of multi-point Padé

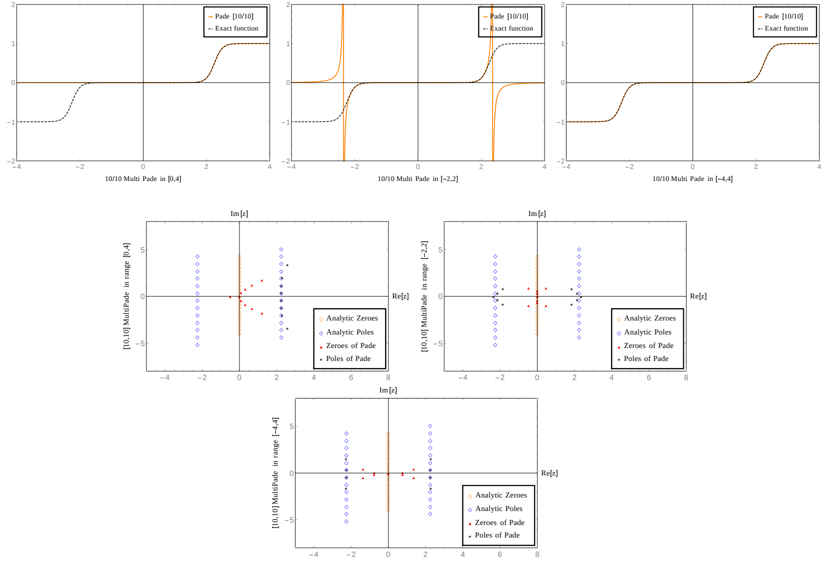
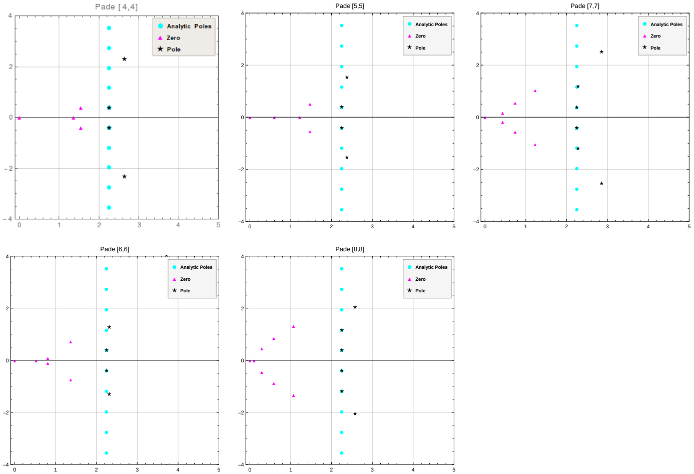


Figure: Depending on what interval we sample points and their Taylor coeffs - we are more (less) sensitive to certain zeroes or poles

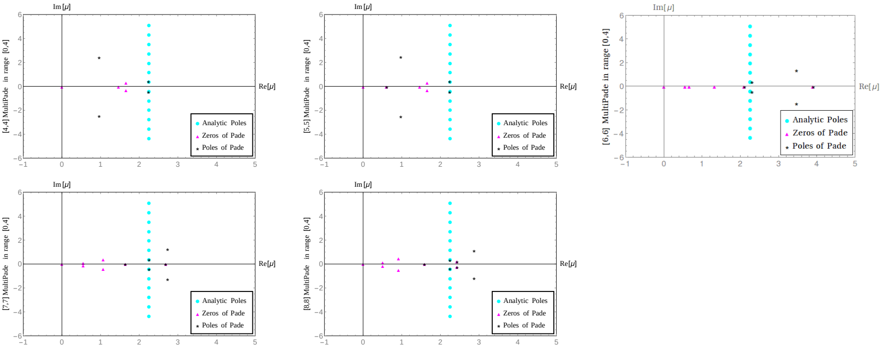
Thirring without errors

- The reconstruction of the line of singularities present in the 1D Thirring model as we increase the order of the approximation. It can be seen that with increasing order the Padé reconstructs more singularities progressively.



Thirring with errors

Performing the exercise above with identical sets of points but now with data that has 1% error on values and 10% error on the first derivatives we get the following picture. It seems that the Padé is able to reconstruct only the closest singularities faithfully. (This is in agreement wit George Bakers book.)



So how bad is the situation?

Figure: Sensitivity to the closest pole even in the presence of errors! Left : 1% noise on values and 10% noise on 1st der and Right : 5% noise on values and 15% noise on 1st der for [4/4] Padé

Figure: Sensitivity to the closest pole even in the presence of errors! Left : 1% noise on values and 10% noise on 1st der and Right : 5% noise on values and 15% noise on 1st der for [6/6] Padé